Development of Dynamical DMRG Method using Regulated Polynomial Expansion and its Application to One-Dimensional Correlated Electron Systems

Shigetoshi Sota, Takanori Sugimoto, and Takami Tohyama

YITP, Kyoto University, Kyoto 606-8502, Kyoto, JAPAN

We have developed a finite temperature dynamical DMRG procedure concentrated on low-temperatures [1] and an effective computational method to calculate a correction vector of the dynamical DMRG [2]. Our finite temperature dynamical DMRG method employs the target state given by the Bolzmann distribution. The target state is calculated by the recursive formula of the regulated polynomial expansion [1, 3]. The correction vector is also calculated by the regulated polynomial expansion. In this method, the δ-functions in the spectrum functions are broaden by a Gaussian. We apply our methods to one-dimensional correlated electron systems. In a spin-1/2 zigzag XY chain, we find that the spin chirality correlation is enhanced by the temperature effect in the dimer phase [4]. Employing a Hubbard-Holstein model, we reproduce the optical conductivity of the Sr_2CuO_3 in the spin excited and the charge-transfer energy region simultaneously as shown in Fig. 1 [2].

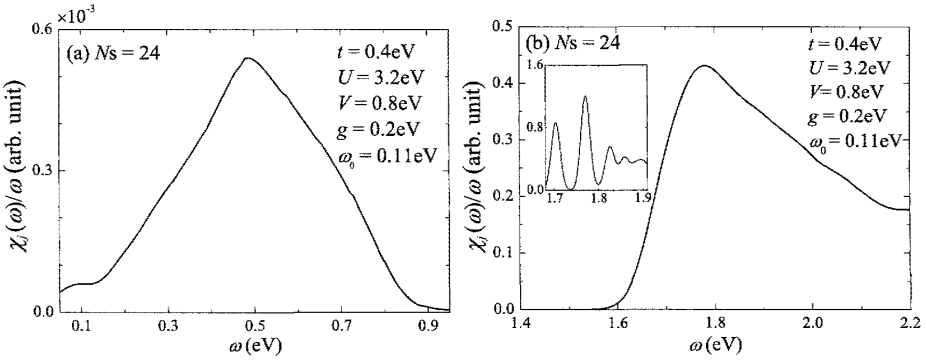

Figure 1: The calculated optical conductivity corresponding to the Sr_2CuO_3.

References

[1] S. Sota and T. Tohyama, Phys. Rev. B **78**, 113101 (2008).

[2] S. Sota and T. Tohyama, arXiv:1007.5166

[3] S. Sota and M. Itoh, J. Phys. Soc. Jpn. **76**, 054004 (2007).

[4] T. Sugimoto, S. Sota, T. Tohyama, Phys. Rev. B **82**, 035437 (2010).